

MODELING OF THE CONTACT REMOVAL OF IRON FROM GROUNDWATER

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Abstract: The paper presents the problem of underwater treatment for drinking water needs. Technological features of water preparation and facilities for its implementation are studied. The model of the removal of iron from water has been developed, mass exchange coefficients have been determined, graphic illustrations of the change of pressure losses and the quality of the filtrate during filtration have been constructed. An algorithm for the solution of a nonlinear regular perturbation problem of the convection-mass transfer type is constructed. A computer experiment based on experimental data has been carried out and the adequacy of the developed model using experimental data was confirmed.

AMS Subject Classification: 65E05, 65M25, 65M32, 68U20, 65C20

Key Words: mathematical model, polystyrene foam filter, water treatment technology, filtering downloading, pressure loss, filtration quality, mass exchange

1. Introduction

In modern society, rational use of water resources in the conditions of water shortage, deterioration of its quality is a complex scientific and technical problem. Water treatment is an important process for water supply. Purification of natural waters, improvement of water preparation technologies and the de-

velopment of new effective resource-saving methods are becoming more and more relevant in recent years. The main purpose of this paper is to investigate the physical and chemical process of contact removal of iron from groundwater and to develop a mathematical model that describes the efficiency of the water treatment taking into account the process parameters. Today about 30% of the total drinking water in Ukraine is drawn from underground sources. There are a wide variety of factors affecting the physical and chemical composition of such water: contact time with different rocks and soils, depth of the media, dissociation in aquifers, contact with the atmosphere and surface waters, etc. For most cases the main problem of groundwater is the high content of iron, hydrogen sulfide and free carbon dioxide (see [1], [2], [3], [4], [6], [7]). In our time there are a wide variety of water treatment methods, which can be grouped as follows: reagent-free; reagent; cation exchange; biochemical (see [3], [4], [5], [6], [12]). One of the simplest and cheapest methods of water treatment is the reagent-free method based on the technology of contact iron removal, which includes simplified aeration of water and subsequent filtration through porous media. This method can be used if the iron content is up to 10 mg / dm³ and the pH is above 7 (see [5]). Contact iron removal is provided by filtration of water with high pH and alkalinity and involves the supply of aeration water immediately to the filters without its preliminary retention (see [1], [2], [3], [4], [7]). The process of iron removal can be carried out with the help of a filter of any design with different granular media - gravel, crushed stone, quartz sand, anthracite, granular plastics, foam polystyrene, etc. The efficiency of water treatment depends strongly on the type of the filter media (see [3], [4], [5]). The technological and design parameters of the filters and their communications are determined at the stage of water treatment plant design. In each case the technology of contact iron removal needs to be specified depending on the physical and chemical parameters of water (see [4], [5], [6], [9]). Treatment of groundwater for meeting regulations is effectively provided at water treatment plants equipped with polystyrene foam filters. One of the possible ways of polystyrene filters optimization is the development of filters based on large-granular media of required fraction obtained at the manufacturing enterprises of polystyrene foam blocks. The advantages of such filters are the small size, cost-effectiveness and high efficiency of groundwater treatment (see [4], [10], [12], [11]).

2. Statement of the problem

The technology of iron removal based on polystyrene foam filters is carried out in the following way. Underground water through pipeline 1 enters the aerator 2, where conversion of divalent iron to the trivalent one, removal of free carbon dioxide and hydrogen sulfide take place. Controller of the filtering speed 3 is designed to remove air bubbles from the water and provide a constant filtering speed throughout the entire filter cycle. From the bottom of the filtering speed controller the water enters the bottom of the filter and runs up through the floating media. The removal of iron hydroxide takes place within the floating polystyrene media. The cleaned water is collected above the filter space and is supplied to the consumer through the pipe 9. When the filter is filled with pollutants the water level in the filtering speed controller is increased and after reaching marginal pressure losses the filter is flushed by opening the valve on the pipeline 10. Cleaned water from above the filter passes through the media extends and flushes it. The flushing water is directed through the pipeline 10 into the sewage system.

In order to improve the organoleptic characteristics of water aeration block is installed in front of the filter unit where in addition to the oxidation of divalent iron removing of the dissolved gases is applied. During the filtration of water containing iron a film appears on filter grains. It has significantly higher sorption properties compared with pure filter. Such a film is regarded as charged and the process of iron removal from the water after the oxidation block takes place as inside of the filter. During filtering compounds of oxidized iron adhere to the surface of the granules with its simultaneous oxidation, that is, the so-called contact iron removal takes place (see [2], [3], [4]). In order to create a mathematical model for describing the physico-chemical processes of removal of iron from water a spatially one-dimensional process of water treatment based on filtration in a polystyrene layer with thickness L (identified with the segment $[0, L]$ along the axis) is considered. According to classical laws mass transfer processes can take place due to diffusion, convection and mass transfer (see [10]). Fick's first law states that

$$q = -D \frac{\partial C}{\partial x} + vC,$$

where q is the "diffusion flux", measures the amount of substance that will flow through a unit area during a unit time interval; D is the diffusion coefficient; C is the concentration (pollution concentration); v is the velocity. For spatial

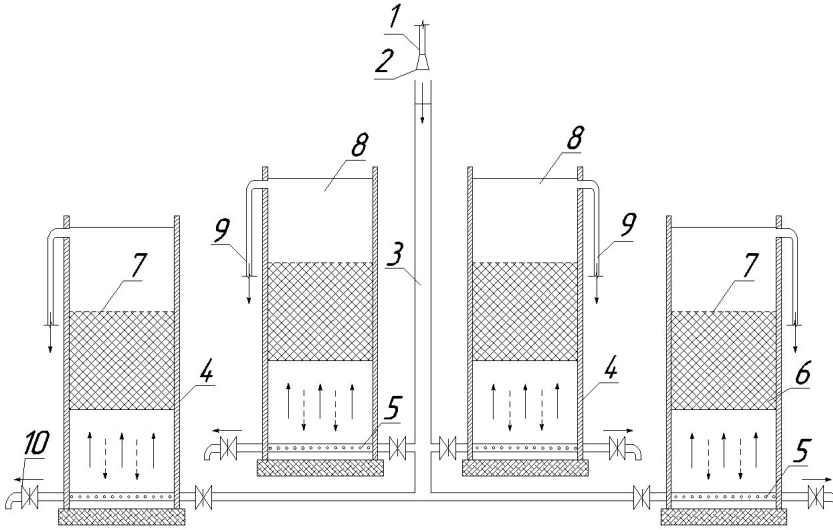


Figure 1: Scheme of iron removal of water by aeration and filtration in polystyrene filters: 1 - pipeline of inlet water; 2 - aerator; 3 - controller of the filtering speed; 4 - filter housing; 5 - distribution system; 6 - floating polystyrene media; 7 - holding screen; 8 - space above the filter; 9 - supplied pipeline of the cleaned water to the consumer; 10 - flushing pipeline

dimensions:

$$q_x = -D \frac{\partial C}{\partial x} + v_x C, q_y = -D \frac{\partial C}{\partial y} + v_y C, q_z = -D \frac{\partial C}{\partial z} + v_z C,$$

$$\frac{\partial q_x}{\partial x} = -D \frac{\partial^2 C}{\partial x^2} + \frac{\partial v_x C}{\partial x}, \frac{\partial q_y}{\partial y} = -D \frac{\partial^2 C}{\partial y^2} + \frac{\partial v_y C}{\partial y},$$

$$\frac{\partial q_z}{\partial z} = -D \frac{\partial^2 C}{\partial z^2} + \frac{\partial v_z C}{\partial z},$$

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = -D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right)$$

$$+ C \frac{\partial v_x}{\partial x} + C \frac{\partial v_y}{\partial y} + C \frac{\partial v_z}{\partial z} + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \pm f(x, y, z, t),$$

where $D = const.$

Taking into account that $\text{div } \vec{v} = 0$ gives

$$\begin{aligned} \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = -D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \\ + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \pm f(x, y, z, t). \end{aligned}$$

According to the expression $\frac{\partial}{\partial \tau} + \text{div } \vec{q} = 0$ we have

$$\begin{aligned} \frac{\partial}{\partial \tau} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \\ - \frac{\partial v_x C}{\partial x} - \frac{\partial v_y C}{\partial y} - \frac{\partial v_z C}{\partial z} \pm f(x, y, z, t). \end{aligned}$$

For liquid treatment the function of sources (inlet-outlet) $f(x, y, z, t)$ defines the following meaning: it characterizes the velocity of sludge accumulation in the filter. From another point of view the amount of sludge captured in the filter is equal to $\frac{\partial \rho}{\partial t} = f(x, y, z, t)$ (ρ is the sludge concentration). Taking into account porosity of the media σ it can be written for one-dimensional case

$$D \frac{\partial^2 C}{\partial x^2} - \sigma \frac{\partial C}{\partial t} - v \frac{\partial C}{\partial x} = \frac{\partial \rho}{\partial t}.$$

This is a differential balance equation. It shows that the amount of matter adhered from liquid within the elementary layer per unit time is equal to that the amount of matter accumulated within this layer per same unit time. Considering the treatment as a result of two opposite effects (adhesion of particles from liquid to the filtering media and avulsion of previously adhered particles due to hydrodynamic flow)

$$\Delta C = \Delta C_1 - \Delta C_2,$$

where ΔC_1 is decreasing of concentration due adhesion; ΔC_2 is increasing of concentration due avulsion. It is accepted that decreasing of concentration due adhesion is proportional to average concentration in elementary volume of the layer

$$\Delta C_1 = \beta C.$$

Increasing of concentration due avulsion of previously adhered particles is proportional to the amount of accumulated sediment in in elementary volume per time unit

$$\Delta C_2 = \alpha \rho,$$

where β, α are filtering parameters which characterize adhesion and avulsion of particles respectively.

So the velocity of sediment accumulation in the filter can be expressed as

$$\frac{\partial \rho}{\partial t} = \beta C - \alpha \rho.$$

Taking into account $D \frac{\partial^2 C}{\partial x^2} - \sigma \frac{\partial C}{\partial t} - v \frac{\partial C}{\partial x} = \frac{\partial \rho}{\partial t}$ and $\frac{\partial \rho}{\partial t} = \beta C - \alpha \rho$ the initial system of equations which describes water treatment is obtained

$$\begin{cases} D \frac{\partial^2 C}{\partial x^2} - \sigma \frac{\partial C}{\partial t} - v \frac{\partial C}{\partial x} = \frac{\partial \rho}{\partial t}, \\ \frac{\partial \rho}{\partial t} = \beta C - \alpha \rho. \end{cases}$$

After multiplying the first and the second equations to $\frac{l}{\beta v}$ and some transformations it is possible to obtain dimensionless equations

$$\begin{cases} \sigma \frac{l}{\beta v} \frac{\partial C}{\partial t} + v \frac{l}{\beta v} \frac{\partial C}{\partial x} + kC - D \frac{l}{\beta v} \frac{\partial C^2}{\partial x^2} = -\frac{l}{\beta v} \frac{\partial \rho}{\partial t}, \\ \frac{l}{\beta v} \frac{\partial \rho}{\partial t} = \beta \frac{l}{\beta v} C - \alpha \frac{l}{\beta v} \rho, \end{cases}$$

$$\begin{cases} \sigma \frac{l}{\beta v} \frac{\partial C}{\partial t} + v \frac{l}{\beta v} \frac{\partial C}{\partial x} + k \frac{l}{\beta v} C - D \frac{l}{\beta v} \frac{l^2}{l^2} \frac{\partial C^2}{\partial x^2} = -\frac{l}{\beta v} \frac{\partial \rho}{\partial t}, \\ \frac{l}{\beta v} \frac{\partial \rho}{\partial t} = \beta \frac{l}{\beta v} C - \alpha \frac{l}{\beta v} \rho, \end{cases}$$

$$\begin{cases} \frac{\sigma}{\beta} \frac{\partial C}{\partial \tilde{t}} + \frac{1}{\beta} \frac{\partial C}{\partial \tilde{x}} + k \frac{l}{\beta v} C - \frac{D}{\beta v l} \frac{\partial C^2}{\partial \tilde{x}^2} = -\frac{1}{\beta} \frac{\partial \rho}{\partial \tilde{t}}, \\ \frac{1}{\beta} \frac{\partial \rho}{\partial \tilde{t}} = \frac{l}{v} C - \frac{\alpha l}{\beta v} \rho. \end{cases}$$

Taking into account $\tilde{t} = \frac{v}{l} t$, $\tilde{x} = \frac{x}{l}$ fields

$$\begin{cases} \frac{\sigma}{\beta} \frac{\partial C}{\partial \tilde{t}} + \frac{1}{\beta} \frac{\partial C}{\partial \tilde{x}} + k \frac{l}{\beta v} C - \frac{D}{\beta v l} \frac{\partial C^2}{\partial \tilde{x}^2} = -\frac{1}{\beta} \frac{\partial \rho}{\partial \tilde{t}}, \\ \frac{1}{\beta} \frac{\partial \rho}{\partial \tilde{t}} = \frac{l}{v} C - \frac{\alpha l}{\beta v} \rho, \end{cases}$$

$$\begin{cases} \frac{1}{s^{-1}} \frac{\partial C}{\partial \tilde{t}} + \frac{1}{s^{-1}} \frac{\partial C}{\partial \tilde{x}} + s^{-1} \frac{m}{s^{-1} \frac{m}{s}} - \frac{\frac{m^2}{s}}{s^{-1} \frac{m}{s} m} \frac{\partial^2 C}{\partial \tilde{x}^2} = -\frac{1}{s^{-1}} \frac{\partial \rho}{\partial \tilde{t}}, \\ \frac{1}{s^{-1}} \frac{\partial \rho}{\partial \tilde{t}} = \frac{m}{s} C - \frac{s^{-1}}{s^{-1} \frac{m}{s}} \rho, \end{cases}$$

$$\begin{cases} \frac{\partial C}{\partial \tilde{t}} + \frac{\partial C}{\partial \tilde{x}} + -\frac{\partial C^2}{\partial \tilde{x}^2} = -\frac{\partial \rho}{\partial \tilde{t}}, \\ \frac{\partial \rho}{\partial \tilde{t}} = C - \rho. \end{cases}$$

Using dimensionless quantities it is possible to identify convective and diffusive contributions to the mass transfer. The value $\frac{D}{\beta vl}$ is equal to $\frac{1}{\beta Pe}$ where Pe is the Peclet number defining the ratio of the convection mass transfer to the diffusive one. Taking into account the values of the corresponding coefficients it is easy to show that the diffusion coefficient can be expressed as $D = b\varepsilon$ and the convective mass transfer one as $\alpha = a\mu$. If $\frac{\varepsilon}{\mu} = \frac{D/\beta vl}{l^2/\alpha} = \frac{D}{l^2\alpha}$ - than $\mu = \varepsilon_*\varepsilon$, $\varepsilon = \frac{D}{\beta vl}$.

Consider a problem describing the filtration process (removal of pollutants from liquid which is characterized by two values of impurity concentrations) according to the classical model (see [8]) taking into account the reverse influence on the porosity and the coefficients characterizing adhesion of impurities and avulsion of sediments. According to the above the mathematical description of this filtering can be written as follows

$$\begin{cases} \frac{\partial \sigma(\rho) c(x, t)}{\partial t} + \frac{\partial vc(x, t)}{\partial x} = -\frac{\partial \rho(x, t)}{\partial t}, \\ \frac{\partial \rho(x, t)}{\partial t} = \beta(\rho) c(x, t) - \varepsilon\alpha(t) \rho(x, t), \end{cases} \quad (1)$$

$$c|_{x=0} = c^*(t), \quad c|_{t=0} = 0, \quad \rho|_{x=0} = 0, \quad \rho|_{t=0} = 0, \quad (2)$$

$$v = \kappa(\rho) \cdot grad p, \quad (3)$$

$$\alpha(t) \int_0^L \rho(\tilde{x}, t) d\tilde{x} = \mu(t), \quad (4)$$

where $c(x, t)$ is the concentration of impurities in liquid; $\rho(x, t)$ is the concentration of impurities deposited in the granular media filter; $\beta(\rho) = (\beta_0 - \beta_*\rho(x, t))v^{\gamma_1}d^{\gamma_2}$ is a function defining mass rate of depositing impurities per unit of time (β_0 is a mass transfer coefficient, β_* is a normalizing coefficient, v is a filtration rate, d is an equivalent diameter of the media, γ_1, γ_2 are empirical coefficients depending on physical and chemical properties of inlet water); $\alpha(t)$ is a function which expresses mass rate avulsed from the granular media filter; $\mu(t)$ is a function defining mass distribution of the sludge during time (is found experimentally (see [8])), condition(4) is supposed for determination $\alpha(t)$ (see [4], [6]);

$c_*^*(t) = C_{in}$ is the concentration of impurities at filter inlet; $\sigma(\rho) = \sigma_0 - \gamma^{-1}\rho$ is the porosity of the filter media (σ_0 is the porosity of the clear media, γ is a mass concentration of solids per unit of volume); $\kappa(\rho)$ is a function defining filtration

$$\kappa(\rho) = \begin{cases} \kappa_0 - \lambda\rho(x, t), & \rho < \rho_0, \\ \kappa_0 - \lambda\rho(x, T_F), & \rho \geq \rho_0, \end{cases} \quad \lambda \text{ is a normalizing coefficient; } \rho_0 = \rho(L, T_F);$$

p is pressure. Unlike to (see [13]) for the more general case the pressure $p = p(x, t)$ should be determined by solving equation $\frac{\partial}{\partial x} \left(\kappa(\rho) \frac{\partial p}{\partial x} \right) = \frac{\partial \sigma(\rho)p}{\partial t}$ which is obtained on the base of the mentioned above equation of continuity and state $div v = \frac{\partial \sigma(\rho)p}{\partial t}$ for boundary $p(0, t) = p_*(t)$, $p(L, t) = p^*(t)$ ($0 < t < \infty$) and initial $p(x, 0) = p_*^*(x)$ ($0 < x < L$) conditions rather smooth and coherent in corner points $G = \{(x, t) : 0 < x < L, 0 < t < \infty\}$ functions are defined. During solving task it is possible to calculate the value of $grad p$, in particular the pressure difference $\Delta P = p^*(t) - p_*(t)$ between the filter inlet and outlet.

3. Methods

Methods of mathematical physics and hydrodynamics were used to build mathematical models of processes of water treatment in which some components dominate others - numerical-asymptotic methods; refinement methodology known classical models by going to the appropriate “perturbed” problems, thus preserving the classic form of laws that describe the processes of fluid flow in porous media, and the construction of their solutions without starting “first” supplement known “unperturbed” solution by various amendments. The modeling is performed in Matlab software using M-function pdepe which solves initial-boundary value problems for systems of parabolic and elliptic partial differential equations (PDE).

4. Results of numerical calculations

Time dependency of mass transfer coefficient $\alpha(t)$ is shown in Figure 1a. Increase of the mass transfer coefficient over time is explained by the fact that during impurity depositing the granules of porous media filter are completely saturated and under hydraulic head the probability of avulsion of particles from granules is increased to time t_3 of effective filtering. The functional dependency of $\beta(\rho)$ and $\alpha(t)$ at filter outlet over time provides evaluation of t_3 (see Figure 2(b)).

Experimental studies of iron removal were performed in laboratory unit with

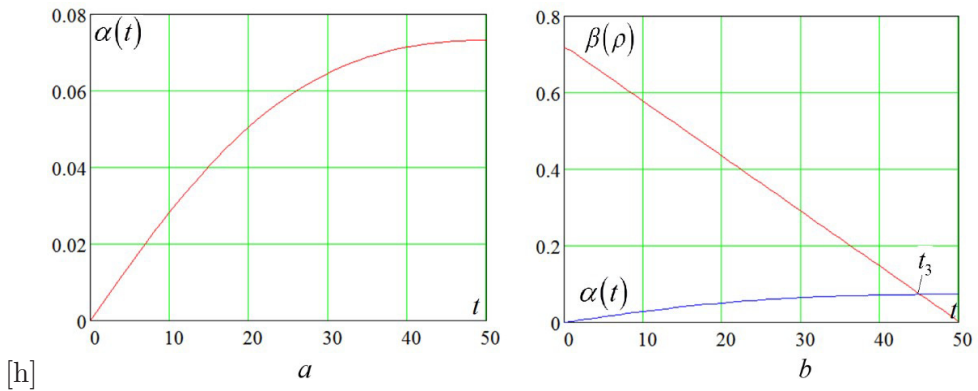


Figure 2: The functional dependency of mass transfer coefficient $\alpha(t)$ (a) and $\beta(\rho)$ with $\alpha(t)$ (b)

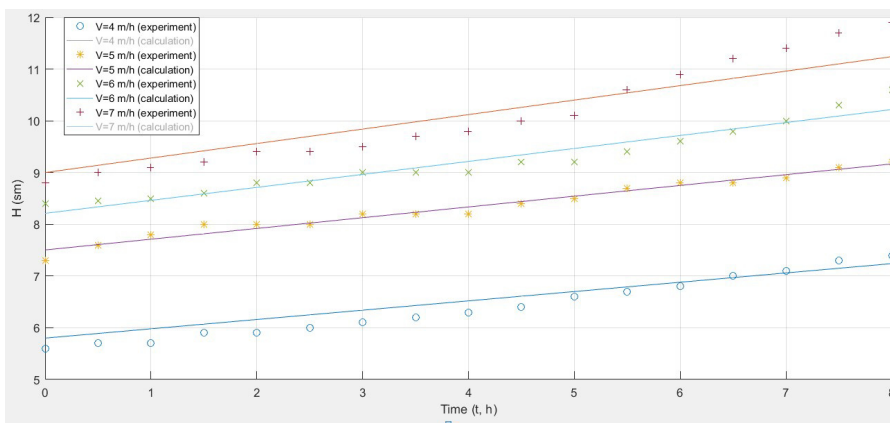


Figure 3: Head drops in the filtering media vs time of filtering graph within the range of filtration velocity 4-7 m/hr and for the concentration of iron 1.5 mg/dm³

modeled water solution. Coarse-grained polystyrene foam of industrial manufacturing is used as a filter media. A series of filter cycles with different inlet concentration of iron in the modeled water solution (1.0...2.0 mg/dm³) were performed for evaluating the statistical relationships of the controlled parameters. The pressure drops studies were carried out within the range of filtration velocity from 4.0 to 7.0 m/hr. Figure 2 shows changes of head drops in the filtering polystyrene media within the range of filtration velocity 4-7 m/hr and for the concentration of iron 1.5 mg/dm³. Data are obtained experimentally

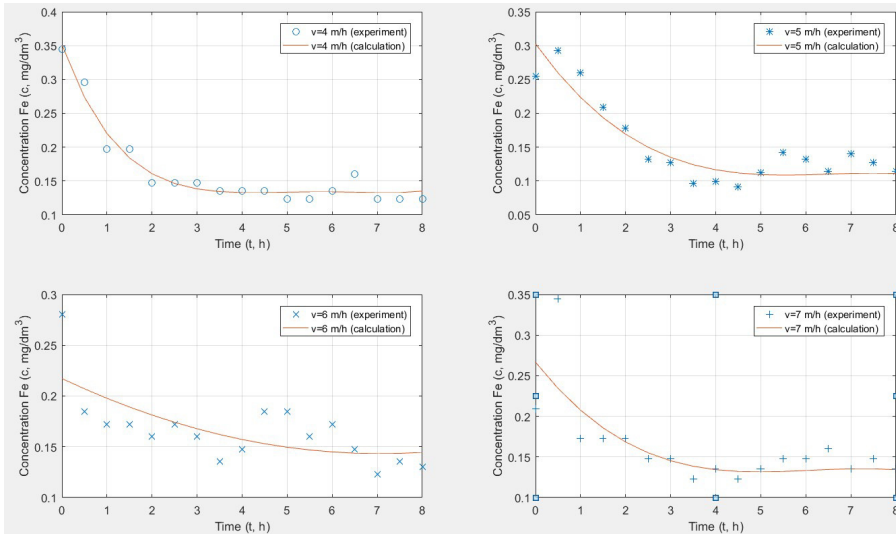


Figure 4: The quality of the filtrate vs the filtration time graph within the range of velocities of 4-7 m/hr and for the iron concentration of inlet water 1.5 mg/dm^3

in the laboratory installation and as a result of a computer experiment solving equations (1) - (3).

The quality of the cleaned water after the iron removal meets the standards requirements of drinking water. The functional relationship between the quality of the cleaned water and the filtration time within the range of velocities of 4-7 m/hr and for the iron concentration of inlet water 1.5 mg/dm^3 was obtained experimentally in the laboratory unit and numerically based on solving (1) - (3). This relationship is presented in Figure 3.

5. Conclusions

A mathematical model that adequately describes the process of removal of iron from water has been developed. The adequacy of the model is experimentally confirmed. The developed model enables to predict changes in head drops with complete and incomplete flush of filter media taking into account the main factors of the process of contact iron removal. The model describes the performance of iron retention within porous media of the filter taking into account parameters of the inlet water.

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